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STRUCTURE OF CHOLESTERYL-4-VINYLBENZOATE

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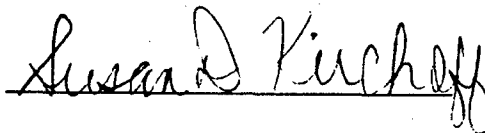
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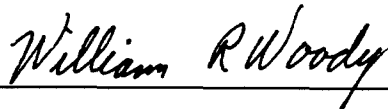
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13. ABSTRACT The structure of cholesteryl-4-vinylbenzoate was determined by X-ray diffraction. The molecule is elongated, with the benzoate group oriented out of the plane of the tetracyclic core. Molecules pack antiparallel, with overlap between either aliphatic tails or tetracyclic cores. These two types of interactions (overlap) are similar to the two packing modes that coexist in the liquid crystalline phase.				
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FOREWORD

The following report was prepared under the AFOSR Summer Research Program under Contract F49620-90-C-0076. The work was initiated under Project No. 2422, "Laser Hardened Materials," Task No. 0401, Work Unit Directive (WUD) 26. It was administered under the direction of the Materials Directorate, Wright Laboratory, Air Force Systems Command, Wright-Patterson Air Force Base, Ohio, with Dr. R.L. Crane as the Materials Directorate Project Scientist (WUD Leader). Coauthors were E. P. Socci and Dr. B. L. Farmer, Dept. of Materials Science and Engineering, University of Virginia, M. L. Chabinyo and Dr. A. V. Fratini, Dept. of Chemistry, University of Dayton, and Drs. T. J. Bunning and W. W. Adams, WL/MLPJ, Wright-Patterson AFB. This report covers the research performed at the Wright Laboratory, Materials Directorate on single crystal X-ray diffraction experiments conducted on in-house synthesized compounds.

Section 1

INTRODUCTION

The Laser Hardened Materials Branch of the Materials Directorate, Wright Laboratory is interested in organic materials with highly ordered molecular structure for nonlinear optical purposes. One class of materials under investigation are thermotropic liquid crystalline compounds, especially those based upon cyclic siloxane backbones.

The first compound exhibiting liquid crystallinity was an ester of cholesterol discovered by Reinitzer in 1888 (Reinitzer, 1888). Since then the liquid crystalline properties of a number of steroidal-based esters (Shibaev & Freidzon, 1989) have been examined. The crystal structures of cholesterol-based materials, most notably those with pendant n-alkanoate ester groups, have also been studied in an attempt to obtain information relating the conformation and packing in the crystalline state to packing in the liquid crystalline phase.

Craven and coworkers (Craven & Guerina, 1979; Guerina & Craven, 1979; Pattabhi & Craven, 1979; Sawzik & Craven, 1979; Sawzik & Craven, 1980a; Sawzik & Craven, 1980b) have observed three distinct packing modes which are dependent upon the length of the pendant n-alkanoate spacer group. Compounds with short spacer lengths (6-8 carbons) exhibit a monolayer structure in which the molecules pack antiparallel. The methyl side groups pendant on the tetracyclic core interlock, leading to efficient packing. Structures of compounds with medium length spacers (9-12

carbons) are comprised of two nonsymmetry related molecules in the unit cell that differ mainly in the conformations of the n-alkanoate groups. The tetracyclic cores in these antiparallel molecules are approximately orthogonal. Compounds with longer spacer groups (13-18 carbons) pack in a bilayer structure in which the molecules are oriented antiparallel. The tetracyclic cores between adjacent molecules do not overlap. Differences in these three packing types have been compared with the variations in packing behavior observed in the liquid crystalline phases (Sawzik & Craven, 1979). Others (Sato & Yano, 1987) have correlated conformations in the crystalline state with the ability of a compound to exhibit liquid crystallinity.

As part of our program aimed toward the development of ordered optically clear thin films, a series of cholesteryl-4-alkenebenzoate materials were synthesized (Bunning, 1992; Gresham, McHugh, Bunning, Klei, Samulski, & Crane, 1993). These compounds were attached to cyclic siloxane backbones. X-ray diffraction measurements of the liquid crystalline phase of these macromolecules indicate the coexistence of two molecular packing schemes (Bunning, Klei, Samulski, Crane, & Linville, 1991; Bunning, Klei, Samulski, Adams, & Crane, 1993). Type I packing consists of nearly fully interdigitated cholesteryl molecules packed antiparallel with a molecular repeat distance (as measured from X-ray diffraction) corresponding to the calculated length of an extended conformation of the molecule. Type II packing consists of antiparallel mesogens packed with overlap only among the aliphatic tails. The relative amounts of type I and II

packing can be controlled by altering several variables including the terminal spacer length. This paper examines the structure of vinylbenzoate substituted cholesterol compounds. Materials with other alkene benzoate spacers are also being studied. Trends in the crystalline packing as a function of alkene-benzoate spacer length may offer insight into the packing behavior in the liquid crystalline phase.

Section 2

EXPERIMENTAL METHODS

The title compound ($C_{36}H_{52}O_2$, F.W.=516.78) was synthesized using a mild esterification reaction of vinylbenzoic acid and cholesterol. Experimental details are available elsewhere (Bunning, 1992). Colorless parallelepiped crystals were obtained by recrystallization from ethyl acetate. A crystal of approximate dimensions 0.37 by 0.30 by 0.27 mm was mounted on a glass fiber with its long axis approximately parallel to the ϕ axis of the goniometer. Preliminary examinations of the crystal and subsequent data collection were performed on an Enraf-Nonius CAD-4 diffractometer equipped with graphite monochromated Mo $K\alpha$ radiation ($\lambda=0.71073$ Å). A rotation (about ϕ) Polaroid was taken and indicated the crystal was of diffraction quality.

Unit cell dimensions were obtained from a least square fit of 25 reflections with $18.02^\circ \leq 2\theta \leq 23.48^\circ$. The orthorhombic cell parameters and calculated volume are: $a=13.755(2)$ Å, $b=24.817(3)$ Å, $c=9.101(2)$ Å, and $V=3101.6$ Å³. There are four molecules per unit cell ($Z=4$).

Intensities were measured at 294 K in a $\omega/2\theta$ scan mode. A total of 5035 reflections in the range of $2^\circ \leq 2\theta \leq 60^\circ$ and $0 \leq h \leq 19$, $0 \leq k \leq 34$, $0 \leq l \leq 12$ were measured. Three intensity monitoring reflections (measured every 120 reflections) showed a decay of 1.79% over approximately 72 hours of data collection. Absorption and decay corrections were applied ($\mu=0.061$). Examination of

reflections for systematic absences led to the choice of space group $P2_12_12_1$ (No. 19).

The phase problem was successfully solved using the direct method program SIR88 (Spagna, R & Viterbo, D., 1989). Structure factors were calculated with scattering factors from the International Tables of X-ray Crystallography (International Tables for Crystallography, 1974). Full matrix least-squares refinement where the minimized function was $\sum w(|F_o| - |F_c|)$ was performed. Nonhydrogen atoms were first refined isotropically and then anisotropically. The 1470 reflections with $F > 2\sigma(F)$ were used in the refinement. Hydrogen atoms were added at calculated positions to the structure model and set as fixed riding atoms. The final cycle of refinement included 243 variable parameters. The final R factor was 0.071 and the weighted R factor was 0.064. The largest shift/error for a parameter was equal to 0.02. All calculations were performed on a Micro-VAX II computer using Enraf-Nonius' MOLEN software. The SYBYL computer modeling program (Tripos Associates, 1991) was used to visualize the molecular packing. A summary of experimental details is given in Table 1. The fractional coordinates and isotropic equivalent temperature factors of the nonhydrogen atoms are listed in Table 2, and anisotropic thermal parameters are listed in Table 3.

Table 1. Experimental Details

Formula	C ₃₆ H ₅₂ O ₂
Formula Weight	516.78
F(000)	1136
Crystal Dimensions	0.37 x 0.30 x 0.27 mm
Radiation	Mo K α
Temperature	294 K
Crystal Form	Orthorhombic
Space Group	P2 ₁ 2 ₁ 2 ₁
Cell Constants	a=13.755(2) Å b=24.817(3) Å c=9.101(2) Å
Volume	3101.6 Å ³
Z	4
Density (calc.)	1.10 g/cm ³
Absorption Coeff.	0.061
Scan type	$\omega/2\theta$
Max 2 θ	59.94°
Reflections Measured	5066 total 5035 unique
Corrections	Lorentz-polarization Numerical absorption (0.9768- 0.9906)
Observations	1470 with $F > 2\sigma(F)$
Parameters	243
R	0.071
wR	0.064
Goodness of fit	1.912
Max shift/error	0.02

Table 2. Fractional Coordinates and Equivalent Anisotropic Thermal
Parameter for Cholesteryl-4-vinylbenzoate

<u>Atom</u>	<u>x</u>	<u>y</u>	<u>z</u>	<u>U_{eq}</u>
O3	0.3961(3)	0.1037(2)	0.4407(5)	5.5(1)
O28	0.2672(3)	0.1459(2)	0.3399(6)	6.4(1)
C1	0.4243(5)	-0.0405(3)	0.3309(9)	5.8(2)
C2	0.4511(5)	0.0178(3)	0.371(1)	6.0(2)
C3	0.3609(5)	0.0523(3)	0.3872(9)	5.0(2)
C4	0.2907(5)	0.0285(3)	0.4934(8)	5.2(2)
C5	0.2676(5)	-0.0305(2)	0.4595(7)	4.0(2)
C6	0.1774(5)	-0.0480(3)	0.4510(8)	4.9(2)
C7	0.1485(4)	-0.1050(3)	0.4282(9)	5.1(2)
C8	0.2313(4)	-0.1445(2)	0.4498(7)	3.6(2)
C9	0.3219(4)	-0.1225(2)	0.3722(8)	3.5(2)
C10	0.3552(4)	-0.0671(2)	0.4400(8)	3.7(2)
C11	0.4032(5)	-0.1639(2)	0.3628(8)	5.0(2)
C12	0.3712(5)	-0.2187(2)	0.3078(8)	4.4(2)
C13	0.2875(4)	-0.2415(2)	0.3994(6)	3.3(1)
C14	0.2055(4)	-0.1997(2)	0.3912(7)	3.7(1)
C15	0.1180(4)	-0.2288(2)	0.4561(8)	4.7(2)
C16	0.1332(4)	-0.2879(3)	0.4098(9)	4.9(2)
C17	0.2346(4)	-0.2917(3)	0.3381(8)	4.3(2)
C18	0.3208(5)	-0.2527(3)	0.5578(7)	5.2(2)
C19	0.4039(5)	-0.0752(3)	0.5871(8)	5.9(2)
C20	0.2809(4)	-0.3478(3)	0.3536(9)	4.7(2)
C21	0.3822(5)	-0.3514(3)	0.290(1)	8.3(3)
C22	0.2148(5)	-0.3906(3)	0.2860(8)	5.5(2)
C23	0.2436(5)	-0.4481(3)	0.3086(9)	6.7(2)
C24	0.1694(5)	-0.4888(3)	0.259(1)	6.6(2)
C25	0.1874(6)	-0.5461(3)	0.275(1)	9.9(3)
C26	0.2671(8)	-0.5670(4)	0.294(2)	27.4(6)
C27	0.1041(7)	-0.5805(3)	0.227(1)	13.1(4)
C28	0.3425(5)	0.1475(3)	0.4059(8)	4.6(2)
C29	0.3908(5)	0.1981(3)	0.4526(7)	4.3(2)
C30	0.4756(5)	0.1980(3)	0.5340(8)	5.2(2)
C31	0.5192(5)	0.2457(3)	0.5715(8)	5.7(2)
C32	0.4818(5)	0.2945(3)	0.5275(8)	4.8(2)
C33	0.3966(5)	0.2944(3)	0.4489(8)	5.4(2)
C34	0.3513(5)	0.2469(3)	0.4125(8)	5.1(2)

Table 2 (con't)

Atom	x	y	z	U _{eq}
C35	0.5325(6)	0.3444(3)	0.5643(9)	6.5(2)
C36	0.5071(6)	0.3936(3)	0.534(1)	7.6(2)
H1A	0.3927	-0.0392	0.2380	7.3*
H1B	0.4813	-0.0618	0.3236	7.3*
H2A	0.4824	0.0168	0.4644	7.9*
H2B	0.4933	0.0336	0.3010	7.9*
H3	0.3273	0.0523	0.2959	6.6*
H4A	0.2324	0.0490	0.4931	6.6*
H4B	0.3202	0.0305	0.5875	6.6*
H6	0.1280	-0.0218	0.4655	6.5*
H7B	0.0978	-0.1132	0.4955	6.5*
H7A	0.1247	-0.1082	0.3305	6.5*
H8	0.2448	-0.1492	0.5513	4.5*
H9	0.3040	-0.1142	0.2738	4.2*
H11A	0.4253	-0.1688	0.4608	6.5*
H11B	0.4551	-0.1512	0.3035	6.5*
H12B	0.3467	-0.2137	0.2110	5.8*
H12A	0.4241	-0.2432	0.3054	5.8*
H14	0.1907	-0.1911	0.2919	4.6*
H15A	0.0592	-0.2144	0.4179	6.3*
H15B	0.1183	-0.2251	0.5600	6.3*
H16B	0.1320	-0.3108	0.4933	6.9*
H16A	0.0835	-0.2984	0.3432	6.9*
H17	0.2345	-0.2882	0.2341	5.3*
H18A	0.3654	-0.2818	0.5622	5.9*
H18B	0.2650	-0.2609	0.6150	5.9*
H18C	0.3507	-0.2210	0.5951	5.9*
H19C	0.4275	-0.0414	0.6208	7.1*
H19B	0.3567	-0.0885	0.6541	7.1*
H19A	0.4562	-0.1000	0.5803	7.1*
H20	0.2868	-0.3532	0.4565	6.9*
H21A	0.3780	-0.3570	0.1873	9.5*
H21B	0.4164	-0.3805	0.3341	9.5*
H21C	0.4158	-0.3187	0.3093	9.5*
H22A	0.2094	-0.3827	0.1841	7.1*
H22B	0.1527	-0.3870	0.3310	7.1*
H23A	0.2597	-0.4547	0.4083	9.3*

Table 2 (con't)

<u>Atom</u>	<u>x</u>	<u>y</u>	<u>z</u>	<u>U_{eq}</u>
H23B	0.2993	-0.4534	0.2488	9.3*
H24B	0.1116	-0.4801	0.3109	9.7*
H24A	0.1590	-0.4839	0.1566	9.7*
H25	0.1862	-0.5489	0.3788	12.4*
H26A	0.3012	-0.5498	0.2165	18.8*
H26B	0.2675	-0.6048	0.2794	18.8*
H26C	0.2913	-0.5630	0.3914	18.8*
H27A	0.1046	-0.6149	0.2722	13.7*
H27B	0.1085	-0.5847	0.1230	13.7*
H27C	0.0454	-0.5623	0.2504	13.7*
H30	0.5025	0.1646	0.5650	6.8*
H31	0.5778	0.2445	0.6267	6.6*
H33	0.3698	0.3277	0.4170	7.4*
H34	0.2911	0.2489	0.3576	7.9*
H35	0.5911	0.3410	0.6188	8.5*
H36A	0.545	0.423	0.559	9.9*
H36B	0.448	0.399	0.477	9.9*

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as: $(4/3) * [a^2*B(1,1) + b^2*B(2,2) + c^2*B(3,3) + ab(\cos \gamma*B(1,2) + ac(\cos \beta*B(1,3) + bc(\cos \alpha)*B(2,3)]$

Table 3: Anisotropic Thermal Parameters for
Cholesteryl-4-vinylbenzoate

<u>Atom</u>	<u>U₁₁</u>	<u>U₂₂</u>	<u>U₃₃</u>	<u>U₁₂</u>	<u>U₁₃</u>	<u>U₂₃</u>
O3	0.071(3)	0.054(3)	0.083(3)	-0.011(3)	-0.020(3)	-0.006(3)
O28	0.072(3)	0.069(3)	0.100(4)	-0.007(3)	-0.034(3)	0.002(3)
C1	0.060(5)	0.059(5)	0.102(6)	-0.015(4)	0.013(5)	0.002(5)
C2	0.075(5)	0.047(4)	0.105(6)	-0.016(4)	0.018(6)	-0.005(5)
C3	0.064(5)	0.061(5)	0.066(5)	-0.006(4)	-0.003(5)	-0.018(4)
C4	0.049(4)	0.075(5)	0.072(5)	0.003(4)	-0.004(4)	-0.003(5)
C5	0.058(4)	0.035(4)	0.061(4)	-0.013(4)	-0.003(5)	0.005(4)
C6	0.048(4)	0.052(4)	0.087(5)	0.009(4)	0.009(5)	-0.004(5)
C7	0.039(4)	0.067(5)	0.088(6)	0.001(4)	-0.003(4)	-0.007(5)
C8	0.043(4)	0.040(4)	0.054(4)	0.003(3)	0.009(4)	-0.002(4)
C9	0.036(3)	0.045(4)	0.052(4)	-0.001(3)	0.004(4)	0.007(4)
C10	0.041(4)	0.049(4)	0.052(4)	0.001(3)	-0.003(4)	0.007(4)
C11	0.047(4)	0.063(5)	0.081(6)	-0.000(4)	0.011(5)	0.007(5)
C12	0.051(4)	0.040(4)	0.076(5)	-0.003(4)	0.018(4)	-0.004(4)
C13	0.043(4)	0.049(4)	0.033(4)	-0.007(3)	0.000(4)	0.006(4)
C14	0.036(3)	0.051(4)	0.052(4)	0.008(4)	-0.011(4)	0.005(4)
C15	0.034(4)	0.063(4)	0.081(5)	-0.001(4)	0.008(4)	0.010(5)
C16	0.040(4)	0.064(5)	0.081(5)	-0.001(4)	0.006(4)	0.015(5)
C17	0.062(4)	0.046(4)	0.057(4)	0.002(4)	0.004(4)	0.005(4)
C18	0.055(4)	0.064(4)	0.078(5)	0.002(4)	-0.013(5)	0.002(5)
C19	0.067(5)	0.066(5)	0.092(6)	-0.005(5)	-0.017(5)	-0.011(5)
C20	0.043(4)	0.058(4)	0.078(5)	-0.013(4)	0.004(5)	0.003(5)
C21	0.077(5)	0.058(5)	0.18(1)	0.003(5)	0.028(7)	-0.005(6)
C22	0.060(5)	0.058(4)	0.092(6)	-0.000(4)	-0.006(5)	0.001(5)
C23	0.097(6)	0.046(4)	0.110(7)	-0.009(4)	-0.029(6)	-0.002(5)
C24	0.067(5)	0.069(5)	0.115(7)	-0.001(5)	0.015(6)	-0.012(6)
C25	0.103(7)	0.058(5)	0.22(1)	0.011(6)	0.004(9)	-0.003(7)
C26	0.36(1)	0.056(6)	0.62(2)	0.056(8)	-0.37(1)	-0.04(1)
C27	0.133(7)	0.088(6)	0.28(1)	-0.069(6)	0.080(9)	-0.049(8)
C28	0.073(5)	0.044(4)	0.057(5)	0.000(4)	0.001(5)	0.008(4)
C29	0.054(4)	0.066(4)	0.042(4)	-0.002(4)	-0.002(4)	-0.007(4)
C30	0.075(5)	0.049(4)	0.074(5)	0.003(4)	-0.006(5)	0.001(5)
C31	0.061(5)	0.079(5)	0.074(6)	-0.004(5)	-0.009(5)	-0.013(5)
C32	0.057(4)	0.063(5)	0.060(5)	-0.009(4)	0.004(4)	-0.012(5)
C33	0.082(5)	0.048(4)	0.075(5)	-0.002(4)	-0.004(5)	-0.007(5)
C34	0.054(4)	0.067(5)	0.074(5)	0.006(4)	-0.018(4)	0.003(5)
C35	0.078(5)	0.073(5)	0.094(6)	-0.013(5)	0.009(6)	-0.020(5)
C36	0.106(6)	0.075(5)	0.108(7)	-0.033(5)	0.009(6)	-0.017(6)

Section 3

DISCUSSION

Bond lengths, bond angles, and torsion angles are compiled in Tables 4, 5 and 6, respectively. A thermal-ellipsoid plot of the molecule (without hydrogen atoms) along with the numbering scheme employed is shown in Figure 1. Bond lengths and angles in the phenyl ring of the benzoate ester compare well with conventional aromatic bond lengths and angles. The benzoate moiety lies out of the plane of the tetracyclic core (illustrated in Figure 2) as indicated by the C2 C3 O3 C28 torsion angle of $152.2(6)^\circ$. The C35-C36 bond length ($1.30(1)\text{\AA}$) is consistent with accepted values for carbon-carbon double bonds, indicating that dimerization did not occur during X-ray exposure. The C28-O28 ($1.199(8)\text{\AA}$) carbonyl and C28-O3 ($1.352(8)\text{\AA}$) ester bonds are in agreement with accepted values. Boat and chair conformations (illustrated in Figure 2) are both present in the tetracycles consistent with results from the n-alkanoate cholesterol series. Large thermal vibrations are observed in the two terminal methyl groups of the aliphatic tail (C26 and C27). In general, the molecule adopts an extended conformation along the b axis.

The antiparallel molecules pack pairwise in the unit cell as shown in Figure 3. Views of the structure along the a, b, and c axes are illustrated in Figures 4-6, respectively. There is a staggered repeat along the a axis of molecules packed with either overlapping aliphatic tails or overlapping tetracyclic cores (Figure 7). The overlapping cores are tilted with respect to each

other. The phenyl ring of the benzoate group lies approximately parallel to the tetracyclic core of the neighboring molecule. The methyl groups of adjacent molecules do not interlock.

The types of interactions exhibited in the solid state have features reminiscent of those observed in the liquid crystalline state (described in the introduction) of cholesterol-4-vinylbenzoate substituted siloxanes. Type I liquid crystalline packing approximates that of antiparallel molecules in the solid state where tetracyclic cores overlap. An end-to-end spacing (along the b-axis) between atoms A and B (shown in Figure 7) of 27.5 Å qualitatively agrees with a 26 Å d-spacing observed for type I packing in the liquid crystalline state. An end-to-end spacing (along the b-axis) between atoms C and D shown in Figure 7 of 45.1 Å qualitatively agrees with an observed (in the liquid crystalline state) type II d-spacing of 47 Å. In the liquid crystalline phase, the amount of type II packing is presumably dictated by steric interactions among aliphatic tails of neighboring molecules. As conditions increase the mobility of the cholesterol molecules (e.g., modification of spacer group length), the amount of type II packing decreases relative to type I packing. We are currently studying the progression of these two packing modes in the crystal structures of cholesterol molecules substituted with longer spacer groups.

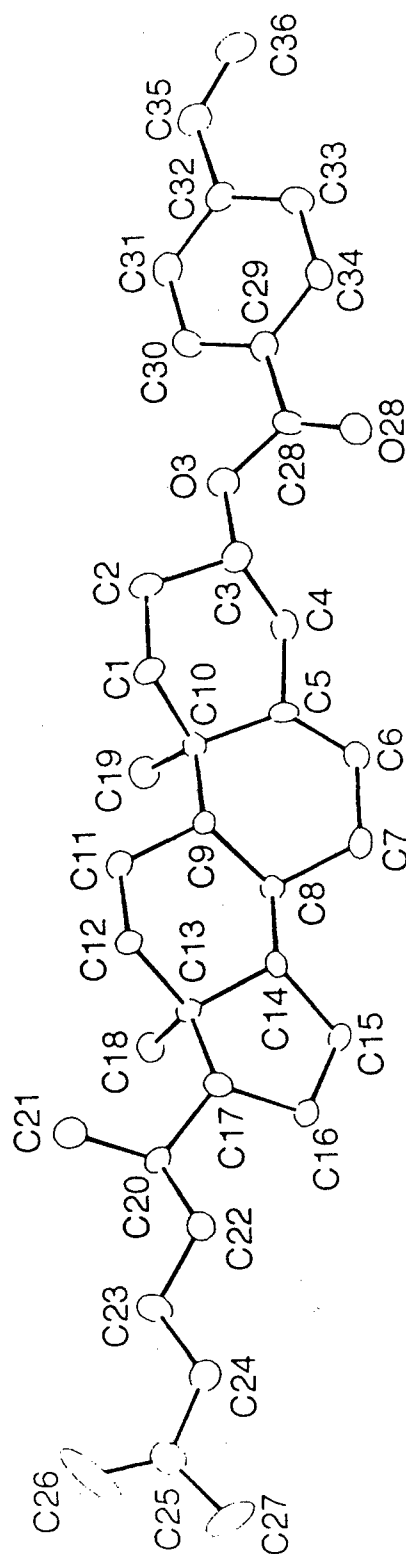


Figure 1: Molecular structure of the title compound along with the atom numbering scheme. H atoms are omitted. Thermal ellipsoids (ORTEP II; Johnson, 1976) are drawn at the 50% probability level.

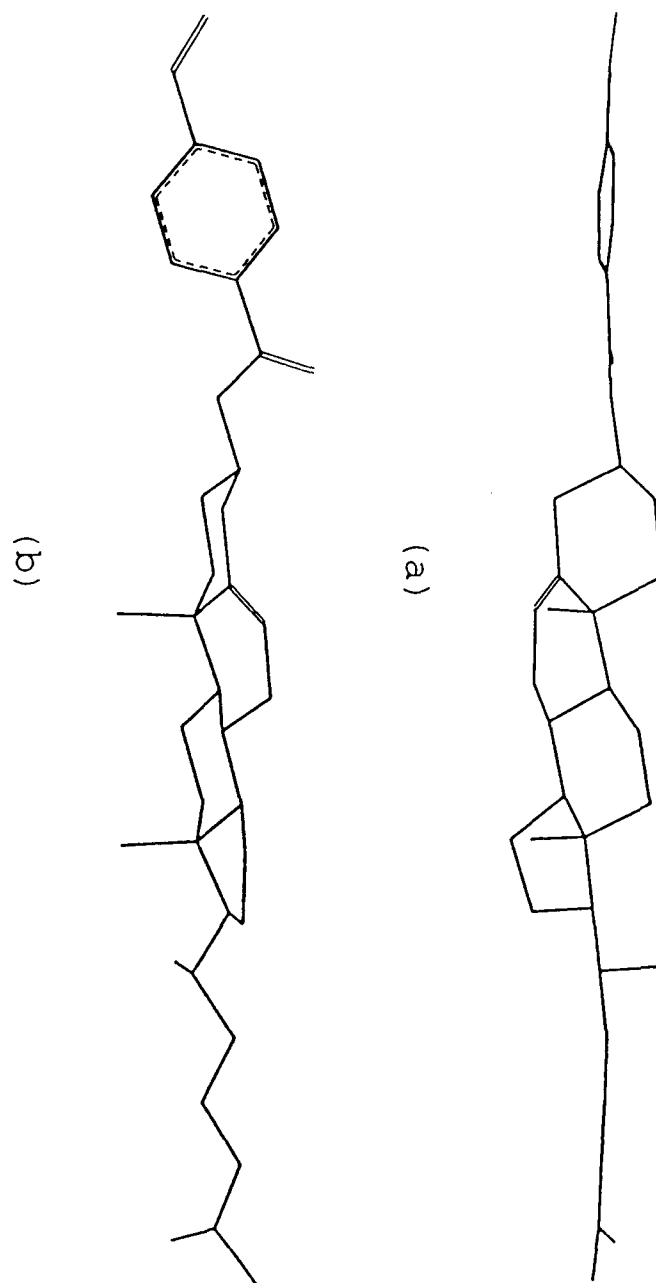


Figure 2: Illustrations showing: (a) the benzoate moiety out-of-plane with the tetracyclic core and (b) boat-chair ring conformations of the tetracyclic core.

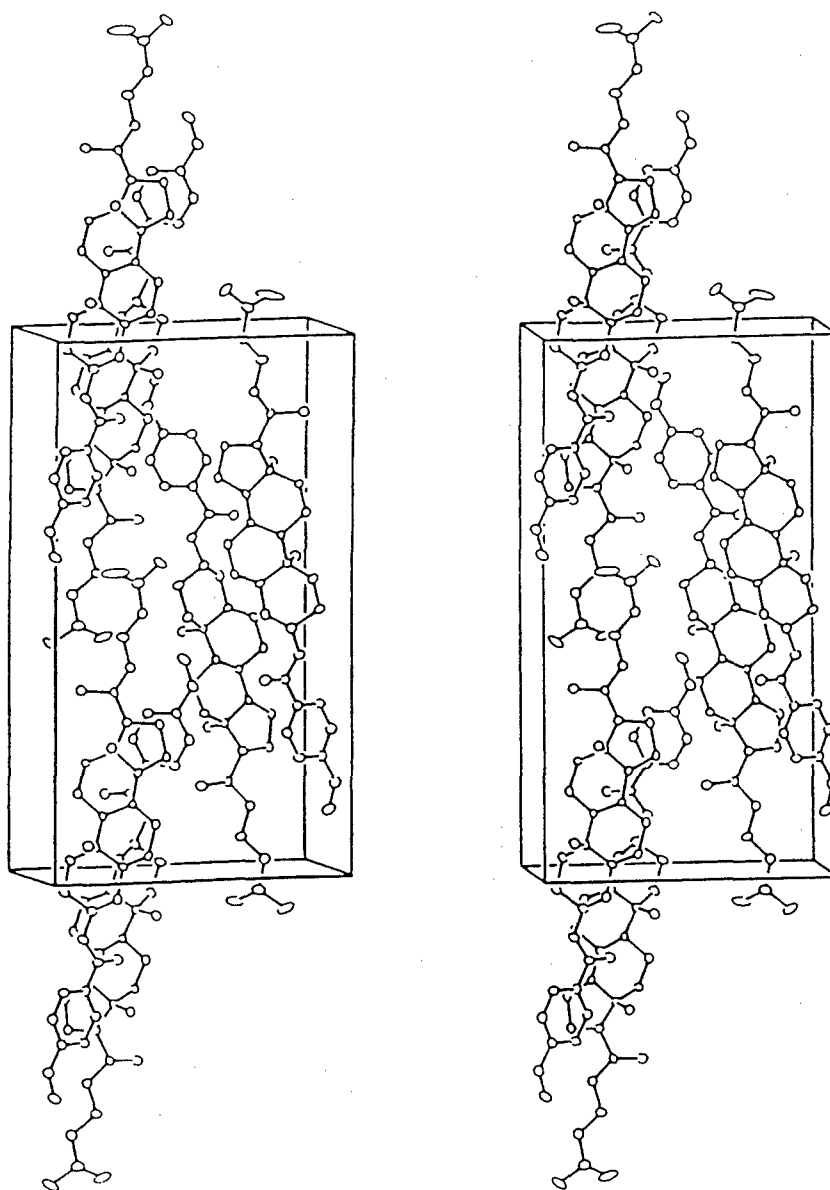


Figure 3: An ORTEPII plot of the unit cell. The c axis is perpendicular to the plane of the paper; the a and b axes are horizontal and vertical, respectively.

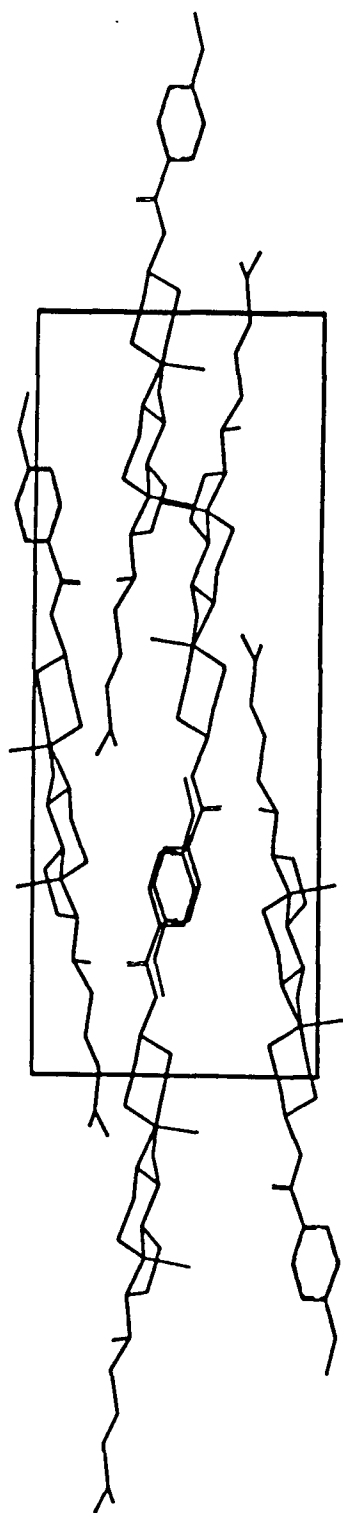


Figure 4: Projection of the crystal structure down the a axis.

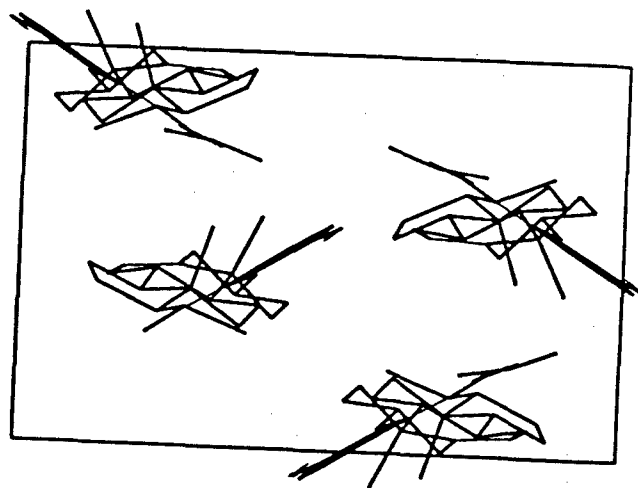


Figure 5: Projection of the crystal structure down the b axis.

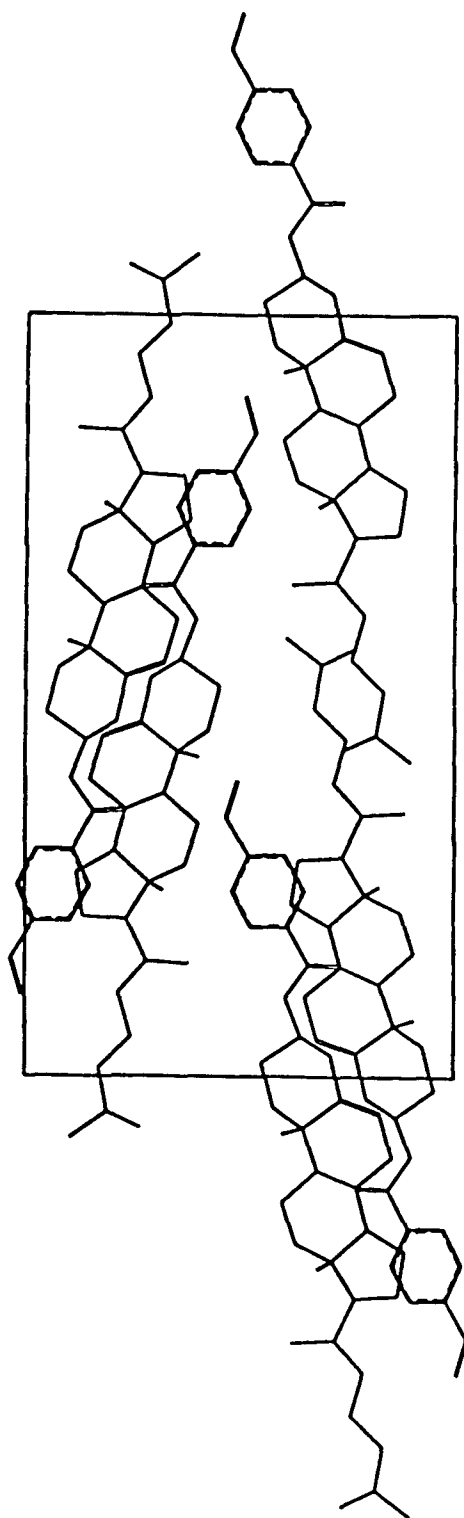


Figure 6: Projection of the crystal structure down the c axis.

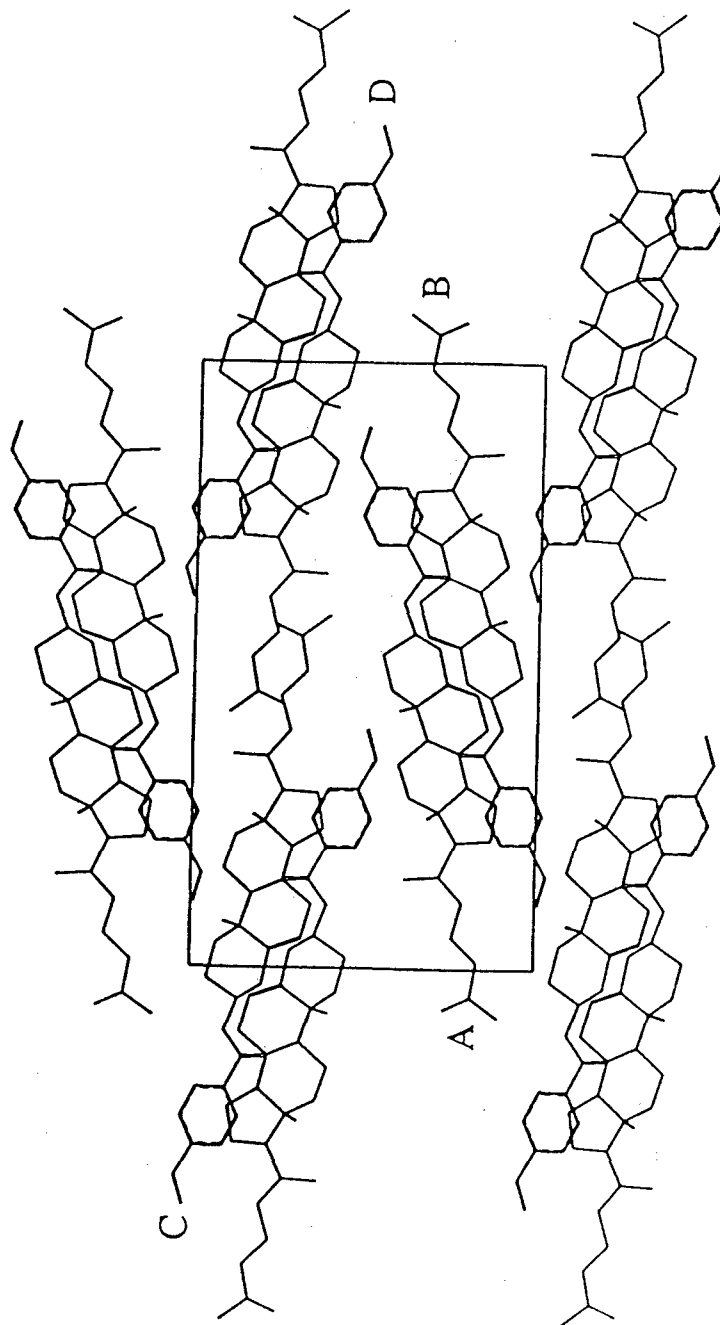


Figure 7: Projection of the cholesteryl-4-vinylbenzoate crystal structure down the c axis. Molecular interaction types are staggered along the a axis. A-B and C-D separation distances are given in the text.

Table 4: Bond Lengths(Å) for Cholesteryl-4-vinylbenzoate

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
O3	C3	1.449(8)	C8	C9	1.534(8)
O3	C28	1.352(8)	C8	C14	1.512(8)
O28	C28	1.199(8)	C8	H8	0.950(7)
C1	C2	1.537(9)	C9	C10	1.574(9)
C1	C10	1.53(1)	C9	C11	1.522(8)
C1	H1A	0.950(8)	C9	H9	0.950(7)
C1	H1B	0.950(7)	C10	C19	1.51(1)
C2	C3	1.515(9)	C11	C12	1.513(9)
C2	H2A	0.950(8)	C11	H11A	0.950(7)
C2	H2B	0.950(8)	C11	H11B	0.950(7)
C3	C4	1.49(1)	C12	C13	1.530(9)
C3	H3	0.950(8)	C12	H12B	0.950(7)
C4	C5	1.528(9)	C12	H12A	0.950(6)
C4	H4A	0.950(7)	C13	C14	1.534(8)
C4	H4B	0.950(7)	C13	C17	1.548(9)
C5	C6	1.317(9)	C13	C18	1.537(9)
C5	C10	1.520(9)	C14	C15	1.522(8)
C6	C7	1.484(9)	C14	H14	0.950(7)
C6	H6	0.950(6)	C15	C16	1.542(9)
C7	C8	1.516(8)	C15	H15A	0.950(6)
C7	H7B	0.950(7)	C15	H15B	0.950(8)
C7	H7A	0.950(8)	C16	C17	1.542(9)
C16	H16B	0.950(7)	C24	C25	1.45(1)
C16	H16A	0.950(7)	C24	H24B	0.950(8)
C17	C20	1.537(9)	C24	H24A	0.950(9)
C17	H17	0.950(7)	C25	C26	1.23(1)
C18	H18A	0.950(7)	C25	C27	1.50(1)
C18	H18B	0.950(7)	C25	H25	0.95(1)
C18	H18C	0.950(7)	C26	H26A	0.95(1)
C19	H19C	0.950(7)	C26	H26B	0.949(9)
C19	H19B	0.950(7)	C26	H26C	0.95(2)
C19	H19A	0.950(7)	C27	H27A	0.950(8)
C20	C21	1.51(1)	C27	H27B	0.95(1)
C20	C22	1.528(9)	C27	H27C	0.950(9)
C20	H20	0.950(8)	C28	C29	1.483(9)
C21	H21A	0.95(1)	C29	C30	1.382(9)
C21	H21B	0.950(7)	C29	C34	1.38(1)
C21	H21C	0.950(7)	C30	C31	1.370(9)
C22	C23	1.494(9)	C30	H30	0.950(7)
C22	H22A	0.950(7)	C31	C32	1.375(9)
C22	H22B	0.950(7)	C31	H31	0.950(7)
C23	C24	1.51(1)	C32	C33	1.37(1)
C23	H23A	0.950(8)	C32	C35	1.46(1)
C23	H23B	0.950(8)	C33	C34	1.37(1)

Table 4 (con't)

<u>Atom 1</u>	<u>Atom 2</u>	<u>Distance</u>	<u>Atom 1</u>	<u>Atom 2</u>	<u>Distance</u>
C33	H33	0.950(7)	C35	H35	0.950(8)
C34	H34	0.968(7)	C36	H36A	0.935(8)
C35	C36	1.30(1)	C36	H36B	0.966(9)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table 5: Bond Angles for Cholesteryl-4-vinylbenzoate

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C3	O3	C28	116.5(5)	C5	C4	H4A	109.8(6)
C2	C1	C10	113.6(6)	C5	C4	H4B	108.9(6)
C2	C1	H1A	107.0(6)	H4A	C4	H4B	109.5(7)
C2	C1	H1B	110.1(6)	C4	C5	C6	121.7(6)
C10	C1	H1A	108.0(6)	C4	C5	C10	115.6(5)
C10	C1	H1B	108.6(6)	C6	C5	C10	122.8(6)
H1A	C1	H1B	109.5(7)	C5	C6	C7	125.2(6)
C1	C2	C3	110.9(6)	C5	C6	H6	116.0(6)
C1	C2	H2A	107.5(6)	C7	C6	H6	118.7(6)
C1	C2	H2B	112.0(7)	C6	C7	C8	113.3(5)
C3	C2	H2A	107.6(7)	C6	C7	H7B	108.2(6)
C3	C2	H2B	109.3(6)	C6	C7	H7A	107.6(6)
H2A	C2	H2B	109.5(7)	C8	C7	H7B	109.2(6)
O3	C3	C2	104.7(5)	C8	C7	H7A	109.0(6)
O3	C3	C4	110.4(6)	H7B	C7	H7A	109.5(6)
O3	C3	H3	117.1(6)	C7	C8	C9	108.7(5)
C2	C3	C4	111.6(6)	C7	C8	C14	111.3(5)
C2	C3	H3	108.4(7)	C7	C8	H8	110.8(6)
C4	C3	H3	104.7(6)	C9	C8	C14	110.6(5)
C3	C4	C5	112.6(6)	C9	C8	H8	109.4(5)
C3	C4	H4A	109.4(6)	C14	C8	H8	106.1(5)
C3	C4	H4B	106.7(6)	C8	C9	C10	111.5(5)
C8	C9	C11	112.4(5)	H12B	C12	H12A	109.5(6)
C8	C9	H9	107.4(5)	C12	C13	C14	106.0(5)
C10	C9	C11	113.5(5)	C12	C13	C17	117.1(5)
C10	C9	H9	104.9(5)	C12	C13	C18	110.7(5)
C11	C9	H9	106.4(6)	C14	C13	C17	100.4(5)
C1	C10	C5	108.1(5)	C14	C13	C18	112.8(5)
C1	C10	C9	107.7(5)	C17	C13	C18	109.4(5)
C1	C10	C19	111.0(5)	C8	C14	C13	115.0(5)
C5	C10	C9	109.7(5)	C8	C14	C15	118.5(5)
C5	C10	C19	109.2(5)	C8	C14	H14	100.5(5)
C9	C10	C19	111.1(5)	C13	C14	C15	104.0(5)
C9	C11	C12	114.4(5)	C13	C14	H14	110.8(5)
C9	C11	H11A	105.6(6)	C15	C14	H14	107.9(5)
C9	C11	H11B	111.1(6)	C14	C15	C16	103.7(5)
C12	C11	H11A	106.8(6)	C14	C15	H15A	110.7(6)
C12	C11	H11B	109.2(6)	C14	C15	H15B	109.8(6)
H11A	C11	H11B	109.5(6)	C16	C15	H15A	111.9(6)
C11	C12	C13	111.7(5)	C16	C15	H15B	111.2(6)
C11	C12	H12B	107.1(5)	H15A	C15	H15B	109.5(6)
C11	C12	H12A	111.1(6)	C15	C16	C17	107.2(5)
C13	C12	H12B	106.6(5)	C15	C16	H16B	110.5(7)
C13	C12	H12A	110.6(5)	C15	C16	H16A	109.8(6)
C17	C16	H16B	108.5(5)	C17	C20	C22	110.2(5)
C17	C16	H16A	111.3(7)	C17	C20	H20	104.8(6)
H16B	C16	H16A	109.5(6)	C21	C20	C22	110.8(6)
C13	C17	C16	102.9(5)	C21	C20	H20	106.7(6)

Table 5 (con't)

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C13	C17	C20	120.1(5)	C22	C20	H20	110.4(6)
C13	C17	H17	106.6(5)	C20	C21	H21A	109.2(7)
C16	C17	C20	113.0(5)	C20	C21	H21B	110.0(7)
C16	C17	H17	114.6(6)	C20	C21	H21C	109.2(7)
C20	C17	H17	100.0(6)	H21A	C21	H21B	109.5(8)
C13	C18	H18A	111.8(6)	H21A	C21	H21C	109.5(8)
C13	C18	H18B	108.2(6)	H21B	C21	H21C	109.5(8)
C13	C18	H18C	108.4(6)	C20	C22	C23	116.8(6)
H18A	C18	H18B	109.5(7)	C20	C22	H22A	107.2(6)
H18A	C18	H18C	109.5(6)	C20	C22	H22B	107.2(6)
H18B	C18	H18C	109.5(6)	C23	C22	H22A	110.5(6)
C10	C19	H19C	108.7(6)	C23	C22	H22B	105.5(6)
C10	C19	H19B	108.3(6)	H22A	C22	H22B	109.5(7)
C10	C19	H19A	111.4(6)	C22	C23	C24	114.8(6)
H19C	C19	H19B	109.5(7)	C22	C23	H23A	111.2(7)
H19C	C19	H19A	109.5(7)	C22	C23	H23B	105.6(6)
H19B	C19	H19A	109.5(7)	C24	C23	H23A	109.1(7)
C17	C20	C21	113.7(5)	C24	C23	H23B	106.4(7)
H23A	C23	H23B	109.5(7)	H27A	C27	H27B	109.5(9)
C23	C24	C25	120.8(7)	H27A	C27	H27C	109(1)
C23	C24	H24B	105.4(7)	H27B	C27	H27C	109(1)
C23	C24	H24A	108.1(7)	O3	C28	O28	124.2(6)
C25	C24	H24B	108.4(7)	O3	C28	C29	111.7(6)
C25	C24	H24A	104.4(8)	O28	C28	C29	124.0(6)
H24B	C24	H24A	109.5(7)	C28	C29	C30	122.0(6)
C24	C25	C26	125.7(8)	C28	C29	C34	119.5(6)
C24	C25	C27	113.6(7)	C30	C29	C34	118.5(6)
C24	C25	H25	99.8(8)	C29	C30	C31	120.2(6)
C26	C25	C27	119.0(8)	C29	C30	H30	119.3(7)
C26	C25	H25	81.(1)	C31	C30	H30	120.5(7)
C27	C25	H25	103.6(8)	C30	C31	C32	121.5(6)
C25	C26	H26A	98.(1)	C30	C31	H31	118.5(7)
C25	C26	H26B	114.(1)	C32	C31	H31	120.0(7)
C25	C26	H26C	114.(1)	C31	C32	C33	118.1(6)
H26A	C26	H26B	109.(1)	C31	C32	C35	120.0(6)
H26A	C26	H26C	118.(1)	C33	C32	C35	121.9(6)
H26B	C26	H26C	103.(1)	C32	C33	C34	120.9(6)
C25	C27	H27A	112.4(9)	C32	C33	H33	119.2(7)
C25	C27	H27B	107.8(9)	C34	C33	H33	119.8(7)
C25	C27	H27C	108.2(8)	C29	C34	C33	120.8(6)
C29	C34	H34	121.4(7)	C36	C35	H35	114.9(7)
C33	C34	H34	117.8(7)	C35	C36	H36A	122.8(9)
C32	C35	C36	128.3(8)	C35	C36	H36B	117.2(8)
C32	C35	H35	116.9(6)	H36A	C36	H36B	119.9(8)

Table 6: Torsion Angles (°) of Cholesteryl-4-vinylbenzoate

<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Atom 4</u>	<u>Angle</u>
C28	O3	C3	C2	152.27(0.60)
C28	O3	C3	C4	-87.47(0.70)
C3	O3	C28	O28	3.18(0.99)
C3	O3	C28	C29	-173.91(0.55)
C10	C1	C2	C3	-56.64(0.83)
C2	C1	C10	C5	52.94(0.73)
C2	C1	C10	C9	171.44(0.53)
C2	C1	C10	C19	-66.76(0.71)
C1	C2	C3	O3	173.89(0.59)
C1	C2	C3	C4	54.45(0.85)
O3	C3	C4	C5	-167.87(0.52)
C2	C3	C4	C5	-51.83(0.78)
C3	C4	C5	C6	-129.74(0.72)
C3	C4	C5	C10	51.60(0.79)
C4	C5	C6	C7	-175.81(0.68)
C10	C5	C6	C7	2.75(1.16)
C4	C5	C10	C1	-50.39(0.75)
C4	C5	C10	C9	-167.59(0.55)
C4	C5	C10	C19	70.46(0.70)
C6	C5	C10	C1	130.97(0.71)
C6	C5	C10	C9	13.77(0.91)
C6	C5	C10	C19	-108.18(0.75)
C5	C6	C7	C8	13.27(1.10)
C6	C7	C8	C9	-44.40(0.81)
C6	C7	C8	C14	-166.44(0.60)
C7	C8	C9	C10	62.06(0.68)
C7	C8	C9	C11	-169.10(0.57)
C14	C8	C9	C10	-175.47(0.50)
C14	C8	C9	C11	-46.63(0.72)
C7	C8	C14	C13	176.28(0.55)
C7	C8	C14	C15	-59.85(0.77)
C9	C8	C14	C13	55.35(0.71)
C9	C8	C14	C15	179.22(0.53)
C8	C9	C10	C1	-163.42(0.51)
C8	C9	C10	C5	-45.98(0.69)
C8	C9	C10	C19	74.83(0.64)
C11	C9	C10	C1	68.35(0.69)
C11	C9	C10	C5	-174.21(0.56)
C11	C9	C10	C19	-53.40(0.73)
C8	C9	C11	C12	48.19(0.80)
C10	C9	C11	C12	175.99(0.56)
C9	C11	C12	C13	-55.02(0.76)
C11	C12	C13	C14	57.57(0.65)
C11	C12	C13	C17	168.53(0.53)
C11	C12	C13	C18	-65.08(0.66)
C12	C13	C14	C8	-59.96(0.67)
C12	C13	C14	C15	168.80(0.51)

Table 6 (con't)

<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Atom 4</u>	<u>Angle</u>
C17	C13	C14	C8	177.73(0.53)
C17	C13	C14	C15	46.50(0.60)
C18	C13	C14	C8	61.37(0.70)
C18	C13	C14	C15	-69.86(0.64)
C12	C13	C17	C16	-154.98(0.53)
C12	C13	C17	C20	78.42(0.75)
C14	C13	C17	C16	-40.82(0.59)
C14	C13	C17	C20	-167.41(0.58)
C18	C13	C17	C16	78.00(0.59)
C18	C13	C17	C20	-48.59(0.75)
C8	C14	C15	C16	-162.43(0.55)
C13	C14	C15	C16	-33.32(0.65)
C14	C15	C16	C17	7.13(0.72)
C15	C16	C17	C13	21.21(0.68)
C15	C16	C17	C20	152.19(0.58)
C13	C17	C20	C21	-55.41(0.88)
C13	C17	C20	C22	179.54(0.57)
C16	C17	C20	C21	-177.16(0.63)
C16	C17	C20	C22	57.79(0.78)
C17	C20	C22	C23	-172.65(0.62)
C21	C20	C22	C23	60.66(0.86)
C20	C22	C23	C24	171.75(0.67)
C22	C23	C24	C25	-179.72(0.83)
C23	C24	C25	C26	-18.06(1.85)
C23	C24	C25	C27	177.21(0.86)
O3	C28	C29	C30	-5.77(0.92)
O3	C28	C29	C34	173.37(0.61)
O28	C28	C29	C30	177.13(0.69)
O28	C28	C29	C34	-3.73(1.07)
C28	C29	C30	C31	178.26(0.65)
C34	C29	C30	C31	-0.88(1.03)
C28	C29	C34	C33	-177.25(0.65)
C30	C29	C34	C33	1.91(1.04)
C29	C30	C31	C32	-1.32(1.09)
C30	C31	C32	C33	2.45(1.07)
C30	C31	C32	C35	-177.43(0.69)
C31	C32	C33	C34	-1.40(1.07)
C35	C32	C33	C34	178.48(0.70)
C31	C32	C35	C36	-178.84(0.84)
C33	C32	C35	C36	1.28(1.31)
C32	C33	C34	C29	-0.77(1.10)

Section 4

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Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	----	-	-	-	----	-----	----
0	4	0	389	381	4	3	3	0	125	125	4
0	6	0	655	636	4	3	4	0	161	150	4
0	10	0	607	605	5	3	5	0	245	232	4
0	12	0	586	557	6	3	6	0	298	289	4
0	16	0	274	257	4	3	7	0	656	652	5
0	18	0	71	87	10	3	8	0	455	458	6
0	20	0	515	509	7	3	9	0	48	49	9
0	22	0	340	337	5	3	10	0	78	73	7
0	28	0	90	80	11	3	11	0	73	87	8
0	34	0	74	12	16	3	12	0	226	211	4
1	3	0	452	446	3	3	15	0	195	201	5
1	4	0	222	222	3	3	16	0	167	167	5
1	6	0	128	125	4	3	17	0	291	290	5
1	7	0	328	326	4	3	18	0	407	415	6
1	8	0	151	155	4	3	19	0	273	262	5
1	10	0	174	175	4	3	20	0	184	184	6
1	11	0	414	388	6	3	22	0	194	199	6
1	12	0	133	118	5	4	0	0	426	436	5
1	15	0	249	251	4	4	1	0	347	349	5
1	17	0	91	99	8	4	2	0	158	160	4
1	19	0	201	198	6	4	3	0	650	664	5
1	20	0	188	197	6	4	5	0	93	99	5
1	21	0	89	79	11	4	6	0	573	573	5
1	22	0	238	254	6	4	7	0	365	381	5
1	23	0	75	113	15	4	8	0	131	146	4
2	0	0	1564	1578	3	4	9	0	139	138	4
2	1	0	451	434	3	4	10	0	320	313	5
2	2	0	491	478	4	4	11	0	276	260	5
2	3	0	452	460	4	4	12	0	114	102	6
2	5	0	159	153	3	4	15	0	85	77	9
2	7	0	96	89	5	4	17	0	104	109	8
2	8	0	224	222	3	4	18	0	211	215	6
2	9	0	272	260	4	4	20	0	116	104	8
2	10	0	806	810	6	4	25	0	69	32	12
2	11	0	1108	1028	6	5	2	0	94	103	5
2	12	0	385	344	6	5	3	0	116	119	5
2	14	0	107	93	6	5	4	0	302	285	5
2	19	0	119	115	8	5	5	0	472	459	6
2	20	0	120	109	9	5	6	0	679	691	6
2	21	0	264	272	5	5	7	0	808	786	6
2	23	0	176	169	6	5	8	0	735	698	6
2	31	0	80	48	14	5	9	0	76	79	8
3	1	0	948	932	4	5	10	0	182	175	4
3	2	0	852	843	4	5	11	0	133	137	5

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	----	-	-	-	----	-----	----
5	12	0	270	275	4	8	12	0	78	51	11
5	13	0	73	76	9	8	13	0	140	150	7
5	16	0	183	186	6	8	14	0	243	251	5
5	17	0	280	284	5	8	16	0	180	186	7
5	18	0	139	144	8	8	20	0	79	51	11
5	19	0	156	165	7	8	24	0	85	78	12
5	20	0	95	81	10	9	1	0	93	81	8
5	30	0	69	17	15	9	2	0	142	154	6
6	0	0	74	80	7	9	4	0	144	130	6
6	1	0	224	217	3	9	5	0	152	138	6
6	2	0	47	50	9	9	6	0	256	246	4
6	3	0	292	275	5	9	7	0	113	131	7
6	4	0	315	314	5	9	8	0	141	137	6
6	5	0	236	234	4	9	13	0	160	143	7
6	6	0	281	280	4	9	16	0	110	114	9
6	7	0	393	394	6	9	20	0	66	76	15
6	8	0	277	283	4	9	22	0	73	49	13
6	9	0	319	299	5	9	28	0	102	63	12
6	11	0	174	172	5	10	0	0	140	129	6
6	13	0	193	184	5	10	1	0	261	250	4
6	14	0	130	137	7	10	2	0	136	139	7
6	15	0	319	316	4	10	6	0	76	44	11
6	16	0	272	272	5	10	9	0	104	112	9
6	17	0	153	141	7	10	10	0	135	141	8
6	18	0	78	77	11	10	11	0	209	207	6
6	19	0	64	62	13	10	13	0	136	142	7
7	3	0	95	91	6	10	14	0	88	103	11
7	4	0	266	252	4	10	26	0	83	59	14
7	9	0	84	81	8	11	2	0	119	119	8
7	13	0	115	117	7	11	4	0	63	61	14
7	15	0	198	188	5	11	5	0	183	186	6
7	16	0	316	310	5	11	6	0	231	238	5
7	20	0	64	81	14	11	7	0	128	119	8
7	26	0	75	69	13	11	8	0	178	186	6
8	0	0	519	502	7	11	9	0	106	106	10
8	2	0	397	411	6	11	11	0	78	70	12
8	4	0	112	108	6	12	0	0	100	97	9
8	5	0	161	170	5	12	1	0	114	109	9
8	6	0	89	103	8	12	2	0	163	168	7
8	7	0	207	214	5	12	4	0	78	83	12
8	8	0	88	93	8	12	5	0	103	111	10
8	9	0	147	141	6	12	7	0	137	148	7
8	10	0	102	117	8	12	9	0	164	175	7
8	11	0	181	185	5	12	10	0	73	71	12

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	-----	-	-	-	----	-----	-----
12	11	0	120	135	9	1	8	1	247	257	4
13	3	0	139	140	7	1	9	1	217	222	3
13	4	0	70	73	12	1	10	1	380	367	5
13	5	0	122	139	9	1	11	1	600	586	6
13	6	0	223	227	6	1	12	1	145	147	4
13	7	0	126	131	8	1	13	1	75	101	8
14	7	0	88	46	10	1	14	1	56	53	10
14	13	0	85	66	12	1	16	1	118	105	6
16	0	0	79	74	13	1	17	1	156	157	6
16	4	0	79	64	13	1	18	1	146	154	6
16	12	0	84	73	14	1	19	1	142	130	7
16	13	0	68	26	15	2	0	1	1401	1477	3
17	12	0	109	83	12	2	1	1	1740	1786	3
18	11	0	99	67	14	2	2	1	268	275	4
0	1	1	272	303	3	2	3	1	433	436	4
0	2	1	360	354	3	2	4	1	280	264	4
0	3	1	156	162	2	2	5	1	260	265	4
0	4	1	413	416	4	2	6	1	172	172	3
0	5	1	461	464	4	2	7	1	256	254	3
0	6	1	594	609	4	2	8	1	186	185	3
0	7	1	180	173	3	2	9	1	250	248	4
0	8	1	511	506	5	2	10	1	187	171	3
0	9	1	162	164	4	2	11	1	373	350	6
0	10	1	188	197	3	2	12	1	245	234	4
0	11	1	359	326	6	2	15	1	73	88	9
0	13	1	262	243	4	2	16	1	97	81	7
0	14	1	154	144	5	2	17	1	101	76	7
0	16	1	236	251	4	2	18	1	237	238	5
0	17	1	82	89	9	2	19	1	162	179	6
0	18	1	155	166	6	2	20	1	93	83	10
0	19	1	182	174	6	2	21	1	228	230	6
0	20	1	122	145	9	2	22	1	161	163	7
0	21	1	196	211	6	3	0	1	201	197	3
0	22	1	195	214	6	3	1	1	548	540	4
0	24	1	69	52	13	3	2	1	661	649	4
0	32	1	75	62	16	3	3	1	287	286	4
1	0	1	253	267	4	3	4	1	406	386	5
1	1	1	910	926	3	3	5	1	401	397	5
1	2	1	169	168	2	3	6	1	193	190	3
1	3	1	432	436	4	3	7	1	228	225	3
1	4	1	335	325	4	3	9	1	260	266	4
1	5	1	289	304	4	3	10	1	512	493	6
1	6	1	472	476	5	3	11	1	247	245	4
1	7	1	173	162	3	3	12	1	277	275	4

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	----	-	-	-	----	-----	----
3	13	1	87	95	7	5	12	1	207	205	4
3	14	1	163	154	5	5	13	1	80	71	9
3	15	1	90	82	8	5	14	1	152	151	5
3	17	1	102	86	8	5	15	1	226	226	5
3	20	1	70	66	12	5	16	1	75	80	10
3	21	1	146	164	7	5	17	1	121	119	7
3	22	1	119	122	8	5	18	1	131	113	8
3	24	1	61	44	13	5	19	1	266	267	5
3	33	1	76	70	16	5	20	1	189	199	6
4	0	1	103	91	5	5	32	1	74	40	15
4	1	1	402	438	5	6	1	1	283	270	4
4	2	1	449	456	5	6	2	1	260	245	4
4	3	1	141	140	4	6	3	1	166	159	4
4	4	1	211	204	3	6	4	1	382	343	6
4	5	1	275	272	4	6	5	1	153	155	4
4	6	1	151	155	4	6	6	1	123	109	5
4	7	1	203	194	3	6	7	1	349	324	5
4	8	1	689	651	6	6	8	1	343	315	5
4	9	1	290	293	4	6	9	1	248	227	4
4	10	1	654	625	6	6	11	1	159	163	5
4	11	1	132	134	5	6	14	1	179	191	5
4	12	1	288	279	4	6	15	1	147	145	6
4	14	1	96	98	7	6	16	1	98	101	9
4	15	1	119	124	7	6	18	1	93	95	10
4	16	1	95	102	8	6	20	1	123	129	8
4	17	1	93	88	9	6	22	1	72	35	12
4	18	1	133	133	7	7	1	1	176	175	4
4	19	1	191	204	6	7	2	1	112	97	6
4	20	1	123	134	8	7	3	1	305	298	4
4	22	1	94	85	10	7	4	1	111	110	6
4	28	1	75	44	13	7	5	1	128	129	5
4	32	1	97	75	13	7	6	1	135	139	5
5	0	1	477	464	5	7	7	1	179	192	4
5	1	1	230	230	4	7	8	1	278	258	4
5	2	1	267	249	4	7	9	1	280	277	4
5	3	1	361	363	5	7	10	1	76	73	9
5	4	1	251	240	4	7	11	1	138	129	6
5	5	1	286	287	4	7	12	1	149	153	6
5	6	1	212	202	3	7	13	1	123	130	7
5	7	1	188	185	4	7	14	1	249	256	5
5	8	1	115	112	5	7	15	1	256	268	5
5	9	1	169	157	4	7	16	1	105	123	9
5	10	1	149	136	5	7	17	1	134	143	7
5	11	1	195	195	4	7	18	1	80	100	11

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	-----	-	-	-	----	-----	-----
7	23	1	66	22	12	11	0	1	80	73	11
7	26	1	75	55	13	11	1	1	90	105	10
8	0	1	219	222	4	11	2	1	110	108	9
8	1	1	159	159	5	11	3	1	179	177	6
8	2	1	259	244	4	11	4	1	184	189	6
8	4	1	94	105	7	11	5	1	181	172	6
8	5	1	108	138	6	11	6	1	91	98	10
8	6	1	74	75	9	11	7	1	163	172	7
8	7	1	93	103	8	11	8	1	77	90	12
8	8	1	128	135	6	11	10	1	142	147	7
8	12	1	91	118	10	11	11	1	85	97	11
8	13	1	98	114	9	11	12	1	145	150	7
8	14	1	268	267	5	11	25	1	72	41	15
8	15	1	288	281	5	12	1	1	78	86	12
8	16	1	173	172	6	12	2	1	127	124	8
8	18	1	105	116	9	12	3	1	146	162	8
8	19	1	133	126	8	12	4	1	115	132	9
8	21	1	91	104	11	12	6	1	73	87	12
9	1	1	73	75	9	12	7	1	124	134	8
9	2	1	104	100	7	12	8	1	100	95	10
9	3	1	109	129	7	12	10	1	241	235	6
9	4	1	152	146	5	12	11	1	86	74	11
9	5	1	136	124	6	12	15	1	77	60	12
9	6	1	184	191	5	13	1	1	85	102	11
9	7	1	112	107	7	13	5	1	66	76	14
9	8	1	84	87	9	13	8	1	76	89	12
9	9	1	170	163	6	13	10	1	97	105	10
9	10	1	121	141	8	13	25	1	89	42	15
9	11	1	81	88	11	14	6	1	64	58	14
9	12	1	102	97	9	14	9	1	110	109	10
9	13	1	172	159	6	15	4	1	69	58	14
9	14	1	121	112	8	16	10	1	92	84	13
9	15	1	128	127	8	16	11	1	90	49	12
9	26	1	99	98	12	0	0	2	1173	1219	4
10	1	1	66	51	11	0	1	2	1079	1146	4
10	2	1	154	157	6	0	2	2	927	949	4
10	3	1	113	120	7	0	3	2	369	357	5
10	6	1	179	179	6	0	4	2	392	394	5
10	7	1	189	196	6	0	5	2	59	73	7
10	8	1	184	194	6	0	6	2	272	276	4
10	9	1	180	182	6	0	7	2	437	438	5
10	11	1	222	231	6	0	8	2	60	53	7
10	12	1	102	89	10	0	10	2	208	202	3
10	26	1	96	69	12	0	11	2	313	306	5

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	----	-	-	-	----	-----	----
0	12	2	49	46	11	2	18	2	179	177	6
0	14	2	212	212	4	2	19	2	259	261	5
0	15	2	225	227	4	2	20	2	166	182	7
0	18	2	226	220	5	2	22	2	239	233	6
0	20	2	131	122	8	3	0	2	136	131	4
0	21	2	100	91	9	3	1	2	955	964	5
0	22	2	159	163	7	3	2	2	489	494	5
0	23	2	91	115	11	3	3	2	487	471	5
0	30	2	109	79	11	3	4	2	260	258	4
1	0	2	2690	2970	14	3	5	2	489	477	5
1	1	2	1582	1678	4	3	6	2	65	66	7
1	2	2	410	430	5	3	7	2	140	154	4
1	3	2	338	341	5	3	8	2	218	222	3
1	4	2	265	267	4	3	9	2	119	118	5
1	5	2	439	439	5	3	10	2	408	394	6
1	6	2	289	288	4	3	11	2	343	325	5
1	7	2	143	146	4	3	12	2	188	186	4
1	8	2	56	57	8	3	13	2	218	219	4
1	9	2	264	270	4	3	14	2	239	247	4
1	10	2	502	486	6	3	15	2	85	93	9
1	11	2	374	359	5	3	16	2	131	123	6
1	12	2	395	404	6	3	17	2	112	110	7
1	13	2	107	104	6	3	18	2	154	164	7
1	16	2	165	178	6	3	19	2	223	237	6
1	20	2	250	258	6	3	20	2	108	111	9
1	23	2	142	150	8	3	21	2	169	178	7
2	0	2	709	716	4	4	1	2	410	434	6
2	1	2	987	1014	4	4	2	2	335	328	5
2	2	2	508	490	5	4	3	2	111	123	4
2	3	2	296	296	4	4	4	2	273	266	4
2	4	2	541	533	5	4	5	2	218	218	3
2	5	2	100	104	5	4	6	2	441	430	6
2	6	2	224	216	3	4	7	2	317	320	5
2	7	2	132	139	4	4	8	2	460	452	6
2	8	2	168	165	4	4	9	2	246	227	4
2	9	2	145	149	4	4	10	2	233	232	4
2	10	2	482	467	6	4	11	2	134	133	5
2	11	2	381	374	6	4	12	2	211	215	4
2	12	2	100	105	6	4	13	2	89	78	7
2	13	2	161	162	4	4	14	2	66	61	10
2	14	2	120	113	6	4	15	2	100	95	8
2	15	2	102	105	7	4	16	2	140	142	6
2	16	2	67	73	11	4	17	2	202	212	6
2	17	2	256	252	5	4	18	2	295	304	5

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	----	-	-	-	----	-----	----
4	19	2	135	138	8	7	9	2	256	257	4
4	20	2	80	56	11	7	10	2	57	51	12
5	0	2	102	116	5	7	11	2	156	150	6
5	1	2	255	238	4	7	12	2	94	97	9
5	2	2	72	88	7	7	13	2	122	122	7
5	3	2	232	224	3	7	14	2	87	92	10
5	4	2	135	133	4	7	15	2	118	106	8
5	5	2	278	268	4	7	16	2	150	142	7
5	6	2	361	331	5	7	17	2	121	120	8
5	7	2	324	313	5	7	26	2	65	35	14
5	8	2	143	139	5	8	0	2	244	237	4
5	9	2	97	106	6	8	2	2	130	130	6
5	10	2	208	210	4	8	4	2	96	110	7
5	11	2	91	85	7	8	5	2	127	124	6
5	12	2	120	115	6	8	6	2	184	180	5
5	16	2	211	213	5	8	7	2	62	67	10
5	17	2	102	100	9	8	9	2	101	85	8
5	18	2	128	136	8	8	10	2	168	170	6
6	0	2	318	321	5	8	12	2	97	91	9
6	1	2	586	577	6	8	13	2	111	113	8
6	2	2	192	195	4	8	15	2	91	87	10
6	3	2	124	119	5	8	16	2	135	151	8
6	4	2	292	288	4	8	22	2	64	30	13
6	5	2	166	165	4	8	30	2	75	47	16
6	6	2	283	271	4	9	0	2	215	207	5
6	7	2	401	408	6	9	3	2	111	110	7
6	8	2	126	135	6	9	4	2	85	68	9
6	10	2	167	164	5	9	5	2	99	83	7
6	11	2	63	73	10	9	6	2	132	140	7
6	12	2	74	53	10	9	7	2	94	91	8
6	14	2	75	58	10	9	8	2	100	110	9
6	15	2	158	177	6	9	9	2	202	211	5
6	16	2	237	248	5	9	10	2	112	135	8
6	17	2	110	127	9	9	11	2	172	169	6
6	20	2	121	115	8	9	12	2	67	87	13
7	0	2	232	241	4	9	13	2	150	172	7
7	1	2	63	81	9	9	14	2	118	119	8
7	2	2	337	316	5	10	1	2	173	175	5
7	3	2	166	164	4	10	2	2	127	121	7
7	4	2	100	99	6	10	3	2	199	198	5
7	5	2	161	162	5	10	4	2	124	123	7
7	6	2	113	94	6	10	5	2	106	118	9
7	7	2	97	98	7	10	6	2	147	164	7
7	8	2	92	115	8	10	7	2	120	116	8

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	----	-	-	-	----	-----	----
10	8	2	140	134	7	0	21	3	137	131	7
10	9	2	97	117	10	0	23	3	151	154	8
10	10	2	113	120	9	1	0	3	219	223	3
10	11	2	100	91	9	1	1	3	440	469	5
10	15	2	126	137	8	1	2	3	604	629	5
11	1	2	108	108	9	1	3	3	142	145	4
11	2	2	175	180	6	1	4	3	103	121	5
11	4	2	87	73	10	1	5	3	138	121	4
11	5	2	106	86	9	1	6	3	184	172	3
11	8	2	125	121	8	1	7	3	220	207	3
11	9	2	82	80	10	1	8	3	251	259	4
11	11	2	90	92	10	1	9	3	146	142	4
12	1	2	84	77	10	1	10	3	92	91	6
12	4	2	139	134	7	1	11	3	257	259	4
12	6	2	170	189	7	1	12	3	316	313	5
12	7	2	151	155	7	1	13	3	152	150	5
12	8	2	133	137	8	1	15	3	109	107	8
12	9	2	120	118	9	1	16	3	136	136	6
12	11	2	113	102	9	1	18	3	136	144	7
13	0	2	97	99	10	1	19	3	86	90	11
13	1	2	71	42	12	1	22	3	73	114	14
13	2	2	69	55	12	2	0	3	384	372	6
13	4	2	94	104	10	2	1	3	329	356	5
13	5	2	93	97	11	2	2	3	484	487	5
13	6	2	101	109	10	2	3	3	256	261	4
14	3	2	89	68	10	2	4	3	291	310	5
14	12	2	74	66	14	2	5	3	160	143	4
14	21	2	99	39	12	2	6	3	72	73	6
0	1	3	866	905	5	2	7	3	118	135	5
0	2	3	116	126	4	2	8	3	176	188	4
0	3	3	106	100	4	2	9	3	117	106	5
0	4	3	144	146	4	2	10	3	472	452	7
0	5	3	70	71	6	2	11	3	169	176	4
0	6	3	110	119	5	2	12	3	143	147	5
0	7	3	58	56	8	2	13	3	69	68	9
0	8	3	56	66	9	2	14	3	54	73	12
0	9	3	494	496	6	2	16	3	91	93	9
0	10	3	202	191	4	2	18	3	97	97	10
0	11	3	523	491	7	2	19	3	146	147	7
0	13	3	74	76	9	2	22	3	89	100	11
0	14	3	60	70	11	2	23	3	95	84	10
0	16	3	97	92	8	3	0	3	575	598	6
0	17	3	144	138	6	3	1	3	480	487	6
0	18	3	163	167	6	3	2	3	443	424	6

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	----	-	-	-	----	-----	----
3	3	3	163	157	4	5	9	3	176	180	4
3	4	3	217	228	3	5	10	3	205	215	4
3	5	3	91	89	5	5	11	3	75	74	9
3	7	3	121	133	5	5	14	3	87	77	9
3	8	3	272	267	4	5	15	3	114	122	8
3	9	3	171	163	4	5	16	3	124	116	8
3	10	3	162	152	5	5	17	3	102	112	9
3	11	3	200	202	4	5	18	3	69	82	12
3	12	3	148	155	5	5	19	3	139	152	7
3	16	3	120	120	7	5	20	3	156	172	7
3	17	3	142	138	7	5	22	3	75	75	12
3	18	3	215	225	6	5	23	3	60	30	14
3	19	3	153	152	7	6	0	3	125	107	5
3	20	3	98	86	9	6	1	3	208	213	4
3	21	3	103	78	9	6	2	3	98	115	6
3	23	3	81	74	11	6	3	3	331	331	5
4	0	3	149	151	4	6	4	3	372	394	5
4	1	3	112	127	5	6	5	3	276	265	4
4	2	3	319	317	4	6	6	3	93	79	7
4	3	3	158	152	4	6	7	3	179	180	5
4	4	3	294	302	4	6	8	3	205	206	4
4	5	3	370	362	5	6	9	3	173	177	5
4	6	3	237	228	4	6	10	3	163	172	5
4	7	3	165	148	4	6	11	3	101	96	7
4	8	3	181	191	4	6	12	3	174	175	5
4	9	3	186	183	4	6	13	3	80	92	10
4	10	3	96	95	6	6	15	3	138	149	7
4	11	3	126	141	6	6	17	3	131	142	7
4	13	3	193	184	5	6	18	3	118	115	8
4	14	3	145	151	6	6	19	3	197	183	6
4	15	3	177	180	5	6	32	3	79	37	15
4	16	3	58	64	13	7	0	3	142	141	5
4	19	3	129	134	8	7	2	3	242	239	4
4	20	3	126	128	8	7	3	3	213	210	4
4	21	3	107	114	9	7	4	3	98	108	7
5	0	3	264	272	4	7	5	3	70	59	9
5	1	3	154	151	4	7	7	3	103	109	7
5	2	3	292	286	4	7	8	3	184	188	5
5	3	3	388	371	6	7	9	3	288	296	4
5	4	3	255	248	4	7	10	3	186	196	5
5	5	3	401	387	6	7	11	3	194	199	5
5	6	3	71	92	8	7	12	3	125	127	7
5	7	3	113	121	6	7	13	3	211	208	5
5	8	3	232	218	4	7	14	3	145	147	7

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	----	-	-	-	----	-----	----
7	15	3	128	140	8	11	3	3	163	164	7
7	16	3	148	156	7	11	4	3	129	132	8
8	1	3	81	72	9	11	6	3	136	133	7
8	2	3	159	167	5	11	10	3	123	135	8
8	3	3	122	135	6	11	12	3	80	78	11
8	4	3	121	124	7	11	14	3	77	84	12
8	5	3	62	54	11	11	16	3	85	72	11
8	6	3	83	91	9	11	18	3	80	42	12
8	8	3	133	148	7	12	3	3	102	108	9
8	9	3	153	166	6	12	4	3	67	39	12
8	10	3	187	184	6	12	5	3	77	76	11
8	11	3	132	124	7	12	9	3	84	90	11
8	12	3	152	152	7	12	20	3	96	89	12
8	13	3	92	92	10	13	0	3	79	61	11
8	14	3	120	124	8	13	2	3	71	64	12
8	15	3	142	166	7	13	3	3	92	78	10
8	21	3	80	67	12	13	4	3	66	79	13
9	1	3	118	118	7	13	6	3	111	102	9
9	2	3	131	136	7	13	10	3	90	96	11
9	3	3	140	160	7	13	17	3	83	63	13
9	6	3	131	127	7	14	4	3	117	100	9
9	7	3	108	120	8	14	5	3	63	55	14
9	8	3	127	114	7	15	6	3	73	72	13
9	9	3	194	217	6	15	10	3	80	97	14
9	10	3	109	98	8	16	6	3	76	37	14
9	11	3	146	143	7	16	8	3	91	27	12
9	13	3	97	108	10	16	11	3	73	42	14
9	14	3	155	173	7	17	6	3	94	41	12
9	15	3	88	73	9	17	10	3	85	88	16
9	26	3	75	27	14	0	0	4	292	296	5
10	1	3	184	191	6	0	1	4	643	657	6
10	2	3	138	138	7	0	2	4	380	382	5
10	3	3	207	221	6	0	3	4	155	160	4
10	4	3	230	231	5	0	4	4	121	121	4
10	5	3	103	101	9	0	5	4	204	208	4
10	7	3	124	127	7	0	8	4	140	140	5
10	8	3	161	156	7	0	9	4	64	58	9
10	10	3	170	189	7	0	10	4	315	331	5
10	12	3	184	194	6	0	11	4	96	90	7
10	14	3	102	100	9	0	12	4	154	150	5
10	15	3	73	61	12	0	13	4	109	88	7
10	22	3	71	43	14	0	14	4	80	83	9
10	24	3	73	58	15	0	15	4	139	138	6
11	2	3	91	117	10	0	19	4	137	139	7

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	----	-	-	-	----	-----	----
0	21	4	145	143	7	3	9	4	219	227	4
0	23	4	159	168	7	3	10	4	206	200	4
0	24	4	81	58	12	3	15	4	79	82	10
1	0	4	268	246	4	3	17	4	131	139	8
1	1	4	355	379	5	3	18	4	105	118	9
1	2	4	73	80	6	3	19	4	153	144	7
1	3	4	165	170	4	3	20	4	115	128	9
1	5	4	223	218	3	3	21	4	134	137	8
1	6	4	102	95	6	3	22	4	99	98	10
1	7	4	90	94	6	3	31	4	78	16	14
1	10	4	118	115	6	4	0	4	137	144	5
1	11	4	117	122	6	4	1	4	112	131	6
1	14	4	69	81	10	4	2	4	172	174	4
1	17	4	174	165	6	4	3	4	148	134	5
1	18	4	63	78	14	4	4	4	168	174	4
1	22	4	86	87	11	4	5	4	251	241	4
1	24	4	66	64	14	4	6	4	127	127	5
2	0	4	215	208	3	4	7	4	178	173	4
2	1	4	345	355	5	4	8	4	113	104	6
2	2	4	657	657	6	4	9	4	188	208	4
2	3	4	155	164	4	4	11	4	117	125	7
2	4	4	246	231	4	4	12	4	79	111	10
2	5	4	163	156	4	4	13	4	122	127	7
2	6	4	63	68	8	4	14	4	114	117	8
2	7	4	222	228	4	4	17	4	131	133	8
2	8	4	183	174	4	4	19	4	130	128	8
2	9	4	97	96	6	4	21	4	119	118	8
2	10	4	152	158	5	4	23	4	80	79	12
2	11	4	162	174	5	4	29	4	67	19	15
2	12	4	124	117	6	5	0	4	381	386	5
2	13	4	124	126	6	5	1	4	538	549	7
2	14	4	141	147	6	5	2	4	245	244	4
2	16	4	150	152	6	5	3	4	73	82	8
2	20	4	122	131	8	5	4	4	162	176	4
2	32	4	74	23	16	5	5	4	90	95	7
3	0	4	365	372	5	5	6	4	110	119	6
3	1	4	750	781	6	5	7	4	116	127	6
3	2	4	222	217	4	5	8	4	225	224	4
3	3	4	324	318	5	5	9	4	126	129	6
3	4	4	157	155	4	5	10	4	127	109	6
3	5	4	86	102	7	5	11	4	217	211	5
3	6	4	151	159	4	5	12	4	125	122	7
3	7	4	128	131	5	5	16	4	89	103	10
3	8	4	101	110	7	5	18	4	99	90	9

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	----	-	-	-	----	-----	----
5	20	4	103	111	9	9	8	4	129	126	7
5	23	4	70	43	12	9	9	4	147	148	7
5	27	4	74	29	14	9	10	4	137	141	7
6	0	4	153	136	5	9	12	4	99	100	9
6	1	4	179	180	5	9	14	4	141	136	7
6	2	4	109	105	7	9	15	4	119	115	8
6	3	4	78	75	8	9	19	4	89	50	10
6	4	4	99	99	7	10	0	4	76	71	11
6	5	4	118	116	6	10	1	4	76	73	12
6	6	4	96	111	7	10	2	4	86	91	10
6	7	4	73	75	10	10	3	4	89	91	10
6	8	4	89	89	8	10	8	4	150	141	7
6	9	4	137	152	6	10	9	4	115	119	8
6	10	4	60	73	12	10	12	4	74	63	12
6	11	4	82	95	10	10	18	4	68	27	13
6	14	4	123	135	8	10	27	4	84	12	14
6	16	4	80	109	11	11	2	4	119	119	8
6	20	4	82	63	10	11	3	4	105	93	8
7	1	4	125	140	6	11	4	4	109	109	9
7	2	4	84	95	9	11	5	4	76	88	11
7	3	4	124	122	6	11	7	4	79	105	12
7	4	4	134	140	6	11	8	4	89	91	10
7	5	4	116	116	7	12	1	4	105	116	9
7	6	4	93	85	7	12	4	4	97	97	11
7	7	4	82	88	10	12	8	4	60	24	13
7	9	4	183	188	5	12	25	4	87	42	14
7	10	4	227	236	5	13	9	4	78	42	12
7	11	4	68	70	12	13	16	4	74	39	13
7	12	4	72	83	12	13	19	4	76	32	14
7	13	4	71	68	12	13	20	4	73	10	15
7	16	4	93	83	9	14	2	4	73	59	13
7	18	4	74	74	11	14	10	4	85	34	12
7	30	4	81	48	15	16	1	4	73	35	14
8	1	4	183	182	5	0	2	5	94	100	6
8	2	4	120	126	7	0	3	5	99	85	6
8	3	4	63	62	11	0	4	5	51	42	10
8	8	4	112	119	8	0	6	5	241	240	4
8	9	4	132	145	8	0	8	5	153	152	5
8	10	4	144	140	7	0	9	5	224	221	4
8	11	4	154	159	7	0	11	5	145	135	6
8	12	4	75	64	12	0	12	5	235	229	5
9	0	4	128	143	7	0	16	5	99	99	9
9	5	4	127	132	8	0	17	5	81	105	11
9	7	4	101	91	9	0	23	5	99	93	10

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	-----	-	-	-	----	-----	-----
1	0	5	406	386	6	4	0	5	178	171	5
1	1	5	210	202	4	4	1	5	177	175	5
1	2	5	169	166	4	4	2	5	202	209	4
1	3	5	242	248	4	4	3	5	137	134	5
1	4	5	104	97	6	4	4	5	194	194	4
1	5	5	110	106	6	4	5	5	179	181	5
1	7	5	99	110	7	4	6	5	112	119	7
1	8	5	123	123	6	4	8	5	213	215	4
1	9	5	164	165	5	4	9	5	97	108	8
1	10	5	141	138	6	4	10	5	177	180	5
1	12	5	77	91	10	4	14	5	71	63	12
1	13	5	106	86	8	4	15	5	75	47	11
1	18	5	67	71	13	4	16	5	109	125	9
1	23	5	108	115	10	4	18	5	62	85	13
2	0	5	160	159	4	4	20	5	88	70	10
2	2	5	386	377	6	5	0	5	349	342	5
2	3	5	126	132	5	5	1	5	200	187	5
2	5	5	100	105	6	5	2	5	164	152	5
2	6	5	115	123	6	5	3	5	99	90	7
2	8	5	192	193	5	5	4	5	142	158	6
2	9	5	182	184	5	5	5	5	145	143	6
2	10	5	163	165	6	5	6	5	132	143	6
2	11	5	162	172	6	5	7	5	54	29	12
2	12	5	187	204	5	5	8	5	97	100	8
2	13	5	80	94	10	5	9	5	125	131	7
2	14	5	67	75	13	5	10	5	85	94	9
2	16	5	124	129	8	5	11	5	76	92	11
2	18	5	171	172	7	5	12	5	122	135	8
3	0	5	93	101	7	5	17	5	128	120	8
3	1	5	190	200	4	5	20	5	176	165	6
3	2	5	162	165	5	6	1	5	125	115	6
3	3	5	189	197	4	6	2	5	77	75	9
3	5	5	154	151	5	6	3	5	108	98	7
3	6	5	147	150	5	6	4	5	173	175	5
3	8	5	183	184	5	6	5	5	78	75	10
3	9	5	144	146	6	6	6	5	114	112	7
3	10	5	248	245	4	6	8	5	147	153	6
3	11	5	104	117	8	6	10	5	173	184	6
3	13	5	109	113	8	6	11	5	198	192	6
3	14	5	64	51	12	6	15	5	92	113	11
3	16	5	70	56	12	6	16	5	139	140	7
3	19	5	99	101	9	7	1	5	152	145	6
3	22	5	100	108	10	7	4	5	139	143	7
3	25	5	74	50	12	7	6	5	96	90	8

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	----	-	-	-	----	-----	----
7	7	5	149	154	7	12	1	5	61	48	13
7	8	5	107	103	9	12	2	5	71	54	12
7	9	5	289	292	5	12	3	5	68	47	12
7	10	5	203	205	6	12	5	5	71	46	13
7	11	5	203	205	6	12	19	5	104	66	11
7	12	5	113	110	8	13	7	5	80	69	13
7	14	5	80	64	11	13	16	5	76	20	14
7	17	5	70	86	13	15	10	5	70	54	16
8	1	5	101	96	9	15	12	5	72	37	15
8	2	5	114	121	8	16	0	5	70	38	15
8	3	5	68	47	12	16	4	5	69	9	15
8	5	5	99	99	9	16	6	5	81	28	14
8	6	5	92	116	11	0	0	6	264	270	4
8	9	5	80	110	12	0	1	6	96	95	7
8	10	5	81	94	11	0	2	6	130	133	5
8	13	5	139	138	7	0	4	6	67	79	9
8	15	5	102	81	9	0	6	6	282	267	4
8	18	5	81	60	11	0	7	6	119	120	7
8	22	5	76	29	13	0	8	6	110	113	7
9	0	5	71	69	12	0	12	6	185	173	6
9	1	5	145	149	7	0	13	6	65	44	13
9	2	5	157	143	6	0	16	6	116	102	9
9	3	5	94	89	9	0	20	6	69	74	12
9	4	5	139	134	7	0	22	6	82	45	12
9	6	5	65	92	12	1	0	6	150	156	5
9	7	5	88	70	10	1	1	6	68	59	8
9	10	5	135	143	7	1	2	6	198	204	4
9	12	5	97	119	10	1	3	6	139	136	5
9	13	5	78	76	12	1	5	6	85	83	8
9	14	5	83	91	12	1	7	6	118	137	7
9	16	5	74	77	12	1	8	6	83	80	9
9	22	5	69	31	14	1	10	6	79	83	10
10	0	5	103	113	9	1	12	6	117	99	8
10	1	5	106	122	9	1	13	6	77	63	11
10	2	5	154	153	7	1	16	6	120	121	8
10	3	5	85	74	11	1	18	6	88	74	10
10	6	5	65	67	13	1	23	6	77	62	13
10	14	5	82	58	12	2	1	6	151	146	5
11	1	5	67	69	13	2	3	6	103	106	7
11	2	5	88	72	9	2	4	6	102	104	7
11	3	5	115	112	8	2	5	6	124	118	6
11	4	5	96	81	9	2	6	6	131	136	6
11	5	5	67	69	13	2	7	6	65	71	11
11	6	5	72	56	12	2	9	6	101	116	8

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	-----	-	-	-	----	-----	-----
2	11	6	111	105	8	6	7	6	93	84	10
2	12	6	64	65	13	6	9	6	80	108	11
2	16	6	105	105	9	6	10	6	140	139	8
2	17	6	126	127	8	6	12	6	139	142	7
3	0	6	73	92	9	6	19	6	74	67	12
3	1	6	252	263	4	7	0	6	217	208	6
3	2	6	246	246	4	7	1	6	141	143	7
3	3	6	69	60	10	7	2	6	115	112	8
3	5	6	180	173	5	7	3	6	82	94	11
3	6	6	122	121	7	7	6	6	85	88	11
3	7	6	134	142	6	7	11	6	76	103	12
3	10	6	91	107	10	7	12	6	98	108	9
3	11	6	104	115	9	7	22	6	77	49	13
3	13	6	77	80	11	8	0	6	65	17	12
3	18	6	70	71	12	8	3	6	74	78	12
3	20	6	62	35	13	8	9	6	177	176	6
3	21	6	83	65	11	8	14	6	67	61	13
4	0	6	303	295	5	9	5	6	66	54	12
4	5	6	95	106	8	9	8	6	83	81	11
4	7	6	209	207	5	9	12	6	65	65	14
4	8	6	73	93	11	10	4	6	64	67	13
4	9	6	107	117	9	10	21	6	86	43	13
4	10	6	91	85	10	10	22	6	89	31	13
4	14	6	77	88	12	11	1	6	75	65	12
4	17	6	84	90	10	11	5	6	75	75	13
4	18	6	65	38	12	11	8	6	79	58	11
5	1	6	129	124	7	14	3	6	68	39	15
5	2	6	73	67	10	14	15	6	86	20	13
5	3	6	107	115	8	0	3	7	83	101	9
5	4	6	76	76	10	0	4	7	113	120	7
5	5	6	113	115	8	0	5	7	157	169	6
5	7	6	92	105	10	0	6	7	126	121	8
5	8	6	134	125	7	0	8	7	125	125	8
5	9	6	203	212	6	0	23	7	66	56	15
5	10	6	153	146	7	1	3	7	133	131	6
5	11	6	146	150	7	1	5	7	92	79	9
5	14	6	112	112	8	1	6	7	89	98	10
5	16	6	74	74	12	1	7	7	131	137	8
6	0	6	225	226	5	1	8	7	92	82	10
6	1	6	203	204	5	1	10	7	82	58	10
6	3	6	100	127	9	1	12	7	73	76	11
6	4	6	126	114	7	2	1	7	96	88	7
6	5	6	90	93	9	2	4	7	87	73	8
6	6	6	77	47	11	2	6	7	113	117	8

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	----	-	-	-	----	-----	----
2	7	7	82	80	11	7	12	7	72	82	14
2	8	7	81	79	10	7	21	7	78	47	14
2	9	7	105	98	9	8	1	7	103	102	10
2	11	7	94	100	10	8	3	7	63	64	13
2	13	7	75	68	11	8	10	7	105	109	9
2	18	7	67	53	14	8	13	7	95	104	11
3	0	7	61	50	12	8	24	7	76	26	16
3	2	7	119	112	8	9	0	7	80	67	12
3	4	7	107	108	8	9	1	7	110	130	9
3	5	7	77	82	11	9	5	7	65	62	13
3	6	7	80	90	11	9	8	7	66	40	13
3	8	7	157	156	7	9	18	7	93	37	11
3	9	7	65	44	13	10	18	7	93	23	12
3	10	7	224	223	6	10	19	7	70	29	16
3	11	7	68	72	12	11	10	7	67	25	14
3	14	7	88	86	10	11	21	7	90	41	14
4	2	7	131	126	8	12	17	7	91	11	12
4	4	7	138	132	7	13	2	7	71	63	15
4	5	7	100	108	9	14	1	7	78	29	13
4	6	7	133	136	7	14	3	7	80	44	14
4	8	7	77	92	12	14	7	7	80	29	14
4	10	7	97	105	9	15	9	7	83	17	15
4	11	7	71	78	12	0	0	8	183	176	6
4	12	7	152	157	7	0	1	8	107	99	8
5	0	7	171	186	7	0	2	8	92	89	9
5	2	7	91	103	10	0	3	8	69	53	11
5	4	7	105	101	8	0	6	8	118	111	8
5	6	7	69	84	12	1	1	8	76	64	10
5	10	7	94	97	10	1	6	8	85	106	10
5	11	7	133	141	8	1	8	8	58	62	13
5	15	7	66	48	13	1	16	8	71	71	13
5	16	7	89	66	11	2	2	8	71	54	9
5	20	7	81	57	12	2	3	8	69	69	10
5	24	7	76	26	14	2	5	8	111	112	8
6	0	7	177	170	6	2	7	8	107	106	8
6	4	7	79	56	11	3	6	8	119	132	8
6	5	7	95	72	9	3	9	8	88	72	10
6	9	7	123	126	8	3	13	8	65	44	13
6	11	7	67	78	14	3	23	8	67	14	15
6	17	7	89	68	11	4	5	8	100	91	9
7	0	7	82	72	11	4	7	8	102	99	8
7	4	7	71	54	12	4	9	8	74	72	11
7	5	7	92	99	10	4	10	8	100	94	9
7	9	7	99	99	10	5	5	8	83	73	10

Appendix

Calculated and Observed Structure Factor Amplitudes for Cholesteryl-4-vinylbenzoate

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
-	-	-	----	-----	-----	-	-	-	----	-----	-----
5	7	8	81	74	11	0	13	10	73	33	14
5	10	8	78	67	11	3	14	10	71	31	14
5	11	8	122	112	8	4	11	10	81	31	13
5	14	8	68	40	14	4	18	10	78	10	14
6	1	8	66	58	13	6	6	10	70	43	14
6	4	8	63	54	13	8	4	10	70	22	15
6	6	8	96	83	10	9	0	10	70	50	15
6	7	8	66	53	13	9	14	10	75	15	16
6	8	8	71	66	13	0	4	11	76	51	13
6	10	8	72	55	13	0	5	11	71	30	13
6	12	8	84	96	12	1	13	11	83	34	13
6	16	8	64	30	14	2	4	11	73	36	13
7	0	8	148	161	8	5	0	11	68	17	14
7	2	8	97	87	10	5	13	11	79	16	15
7	9	8	97	83	10	7	11	11	75	5	15
7	11	8	81	28	11	8	1	11	76	13	15
8	0	8	98	96	10	9	1	11	77	15	15
8	1	8	104	81	9	0	4	12	67	12	15
8	2	8	64	44	14						
8	6	8	80	66	12						
9	5	8	68	14	13						
9	19	8	74	25	16						
10	2	8	83	45	11						
0	2	9	62	31	11						
0	3	9	74	85	11						
0	5	9	94	73	9						
0	7	9	65	77	13						
1	4	9	101	106	9						
1	8	9	80	85	11						
1	9	9	69	58	13						
2	8	9	63	65	13						
2	22	9	81	31	14						
3	10	9	82	84	12						
3	12	9	96	85	11						
3	16	9	79	6	13						
3	22	9	72	15	14						
4	11	9	94	90	11						
5	2	9	76	48	11						
5	8	9	68	50	13						
6	12	9	73	21	13						
10	0	9	79	17	13						
10	4	9	89	51	12						
12	10	9	82	22	15						
13	1	9	78	40	15						